

Density-functional theory for the pairing Hamiltonian

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We consider the pairing Hamiltonian and systematically construct its density functional in the strong-coupling limit and in the limit of large particle number. In the former limit, the functional is an expansion into central moments of occupation numbers. In the latter limit, the functional is known from BCS theory. Both functionals are nonlocal in structure, and the nonlocalities are in the form of simple products of local functionals. We also derive the relation between the occupation numbers and the Kohn-Sham density.

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I. INTRODUCTION

Density-functional theory (DFT) is a very popular theoretical method in many branches of physics, as it allows one to obtain the ground-state energy of an interacting many-fermion system from the solution of a mean-field equation [1, 2]. The main challenge in DFT is the connection between the Hamiltonian and the form of the density functional. Usually, one approximates the unknown (and supposedly nonlocal) density functional in terms of local densities, currents, and gradients of the density. This approach has led to impressive results in quantum chemistry [3] and nuclear physics [4, 5, 6, 7].

Pairing plays an important role in atomic nuclei (see, e.g., Ref. [8] for a recent review). Within the mean-field approach to nuclear structure, pairing is often included in the form of the BCS model added to the Skyrme functional [9], or through Hartree-Fock-Bogoliubov (HFB) calculations [10, 11]. The formal extension of Kohn-Sham DFT to superconductors also leads to HFB equations [12]. In these latter two approaches, the energy is a functional of the density and the pairing field (anomalous density). It is thought that the latter is a highly nonlocal functional of the density and thereby captures aspects of the density functional that would be difficult to model otherwise. Within the HFB approach, the particle number is not a conserved quantity anymore, and particle number projection becomes a concern and additional expense [13]. In this work, we revisit the pairing problem and construct its density functional without resorting to the HFB approach. We thereby avoid some of the problems associated with pairing fields and gain insight into the nonlocal structure of the density functional.

The direct and systematic construction of a density functional from a given Hamiltonian is possible only for solvable or sufficiently simple systems. We mention, for instance, the systematic construction of the density functional for a dilute Fermi gas with repulsive interactions [14, 15], or the description of the Fermi gas close to the unitary limit in terms of local densities [16] and gradient corrections [17, 18]. Albeit being simple, these systems are nontrivial, and they provide us with useful insights

for the empirical construction of the nuclear density functional. Examples are, e.g., the occurrence of terms proportional to $\rho^{7/3}$ [14] or proportional to $\rho^{5/3}$ [17] which are absent in presently employed functionals. The pairing Hamiltonian is another solvable problem, and the derivation of its density functional is the purpose of this paper.

This paper is organized as follows. In Sect. II, we describe the pairing Hamiltonian and the method to derive its density functional. In Sect. III, we construct the density functional in the limit of large numbers of pairs. In Sect. IV, we construct the density functional in the limit of large coupling strength. Both density functionals will be given in terms of occupation numbers. In Sect. V, we work out the relation between occupation numbers and the spatial density, and discuss extensions of presently employed density functionals to include pairing. We close with a summary of our results.

II. HAMILTONIAN AND METHOD

The pairing Hamiltonian is defined as

$$H = \sum_{j=1}^{\Omega} \sum_{s=\downarrow, \uparrow} \varepsilon_j \hat{a}_{js}^{\dagger} \hat{a}_{js} - g \sum_{i,j=1}^{\Omega} \hat{a}_{i\downarrow}^{\dagger} \hat{a}_{i\uparrow}^{\dagger} \hat{a}_{j\uparrow} \hat{a}_{j\downarrow}. \quad (1)$$

We thus have Ω single-particle orbitals which can be doubly occupied with a constant pairing interaction. This pairing model was studied and solved by Richardson in the 1960s as an alternative to the BCS approximation [19]. Recently, the Richardson model has found renewed interest in the framework of superconductivity in small mesoscopic systems, and we refer the reader to the review by Dukelsky *et al.* [20]. The Hamiltonian (1) is exactly solvable and integrable (i.e., there are as many conserved quantities as degrees of freedom [21]). The ground-state energy

$$E = 2 \sum_{i=1}^N E_i \quad (2)$$

of N pairs of fermions is given in terms of the solutions E_i of the Richardson equations

$$\sum_{j=1 \atop (j \neq i)}^N \frac{2}{E_i - E_j} = \frac{2}{g} + \sum_{k=1}^{\Omega} \frac{1}{E_i - \varepsilon_k} \quad i = 1, \dots, N. \quad (3)$$

Note that the ground-state energy (2) depends implicitly on the single-particle energies ε_k . Note also that the ground state of the pairing model is a superposition of fully paired states, since singly occupied orbitals are not subject to the interaction.

We want to construct the density functional for the pairing Hamiltonian. This requires us to compute the Legendre transform

$$F(\{n_k\}) = E - \sum_{k=1}^{\Omega} n_k \varepsilon_k \quad (4)$$

of the ground-state energy (2) with respect to the occupation numbers

$$n_k \equiv \frac{\partial E}{\partial \varepsilon_k}. \quad (5)$$

Due to the Hellman-Feynman theorem, the occupation numbers (5) are indeed the expectation value $n_k = \langle \psi | (\hat{a}_{k\downarrow}^\dagger \hat{a}_{k\downarrow} + \hat{a}_{k\uparrow}^\dagger \hat{a}_{k\uparrow}) | \psi \rangle$ of the ground-state $|\psi\rangle$. Usually, DFT practitioners work with the density instead of occupation numbers. However, the Hamiltonian (1) is given in terms of the Fock-space operators \hat{a}_k^\dagger and \hat{a}_k , and its density functional is therefore naturally expressed in terms of occupation. The relation between the density and the occupation numbers will be given in Sect. V.

In order to actually perform the Legendre transform (4), we need a closed expression of the ground-state energy in terms of the single-particle energies. Unfortunately, no such expression is available for the solutions of the Richardson equations (3), as these equations have to be solved numerically [22, 23]. However, closed expressions for the ground-state energy do exist for the two limiting cases of a large number of pairs $N \gg 1$ or a large coupling strength $g/\varepsilon_k \gg 1$. In Sect. III and Sect. IV, we will construct the density functional of the pairing Hamiltonian in these two limits, respectively.

Note that the density functional is only determined up to an overall constant. Shifting the single-particle energies ε_k by a constant does not change the corresponding occupation numbers n_k . Indeed, summing Eq. (5) over k yields $\sum_{k=1}^{\Omega} n_k = 2N$, which is independent of the single-particle energies ε_k . Thus, it is not possible to invert the equations (5) and to express the single-particle energies in terms of the occupation numbers. To avoid this problem, one can introduce an orthogonal transformation from the single-particle energies ε_k to new variables e_1, \dots, e_{Ω} such that $e_1 = (1/\sqrt{\Omega}) \sum_{k=1}^{\Omega} \varepsilon_k$. The new variables e_2, \dots, e_{Ω} are invariant under a constant shift of the single-particle energies ε_k (since they are orthogonal to e_1). The corresponding new occupation numbers $\nu_k = \partial E / \partial e_k$ are related to the occupation numbers

n_k by the same orthogonal transformation. One has in particular $\nu_1 = 2N/\sqrt{\Omega}$ and $F(\{\nu_k\}) = E - \sum_k \nu_k e_k$. The inversion can be performed for the new variables e_2, \dots, e_{Ω} . Note that variations of the resulting density functional $F(\{\nu_k\})$ with respect to $\nu_2, \dots, \nu_{\Omega}$ conserve the number of particles.

For the cases considered in Sect. III and in Sect. IV, respectively, we can follow a simpler path. The ground-state energy depends only on certain combinations of single-particle energies. These can directly be expressed in terms of combinations of occupation numbers without solving the individual ε_k in terms of the n_k .

III. DENSITY FUNCTIONAL IN THE LIMIT OF LARGE PARTICLE NUMBER

In the limit of a large number of pairs $N \gg 1$, the Richardson equations (3) can be solved in a systematic expansion [24, 25]. This leads to the BCS energy

$$E_{BCS} = \sum_{k=1}^{\Omega} \varepsilon_k - \mu(\Omega - 2N) + \frac{\Delta^2}{g} - \sum_{k=1}^{\Omega} \sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}. \quad (6)$$

The gap Δ and the chemical potential μ determined by

$$\frac{2}{g} = \sum_{k=1}^{\Omega} \frac{1}{\sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}}, \quad (7)$$

$$\Omega - 2N = \sum_{k=1}^{\Omega} \frac{\varepsilon_k - \mu}{\sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}}. \quad (8)$$

We are interested in the construction of the density functional for the pairing Hamiltonian with ground-state energy (6) and perform the Legendre transform (4) in three steps. First, we compute the occupation numbers

$$n_j = \frac{\partial E_{BCS}}{\partial \varepsilon_j} = 1 - \frac{\varepsilon_j - \mu}{\sqrt{(\varepsilon_j - \mu)^2 + \Delta^2}}. \quad (9)$$

Here, we made use of Eqs. (8) and (7). The form Eq. (9) is intuitively clear: For vanishing gap, the occupation numbers are two and zero for orbitals below and above the chemical potential, respectively. Second, we invert this equation and obtain the single-particle energies as a function of the occupation numbers

$$\varepsilon_j = \mu + \frac{(1 - n_j)\Delta}{\sqrt{n_j(2 - n_j)}}. \quad (10)$$

Here, the gap and the chemical potential are also functions of the occupation numbers. Indeed, summing Eq. (9) over all orbitals yields Eq. (8), while we obtain

$$\Delta = \frac{g}{2} \sum_{j=1}^{\Omega} \sqrt{n_j(2 - n_j)} \quad (11)$$

from the gap equation (7). Third, we compute the Legendre transform and obtain the density functional

$$\begin{aligned} F_{BCS} &\equiv E_{BCS} - \sum_{j=1}^{\Omega} \varepsilon_j n_j \\ &= -\frac{\Delta^2}{g} \\ &= -\frac{g}{4} \left(\sum_{j=1}^{\Omega} \sqrt{n_j(2-n_j)} \right)^2. \end{aligned} \quad (12)$$

The equations presented in this section are well known from BCS theory [9, 26]. The form of the functional clearly exhibits two properties of the pairing interaction. (i) Pairing creates an instability of the Fermi surface, and (ii) is nonanalytical for weak couplings. Property (i) is included in the functional (12) as there is a gain of energy associated with deviations of the occupation numbers from two and zero. Property (ii) is also fulfilled since the functional is nonanalytical for small values of $2 - n_k$ and n_k , respectively. Note that the functional is nonlocal, as it is the square of a local functional. Note also that the functional (12) is among the simplest ones that includes nonlocality, overall quadratic scaling in occupation numbers (motivated by a two-body interaction), and properties (i) and (ii). From this point of view, the form of the functional could almost have been guessed.

IV. DENSITY FUNCTIONAL IN THE STRONG-COUPLING LIMIT

Pairing in nuclei is often associated with the weak-coupling regime. An exception are, e.g., nuclei with magic proton number where the neutrons partly fill a single j -shell. For such nuclei, pairing is dominant due to the degeneracy of the single-particle orbitals. We consider the corresponding strong-coupling regime in this section and gain additional insight in the nonlocal structure of density functional.

Within the strong-coupling regime, the ground-state energy can be computed within the quasi-spin formalism [27]. Here, we follow approach by Yuzbashyan *et al.* [25]. In the strong-coupling limit, the pairing term is the dominant part of the Hamiltonian (1), and one has $g \gg |\varepsilon_k - \bar{\varepsilon}|$. Here, and in what follows, we denote averages over single-particle orbitals by the overbar, e.g.

$$\bar{\varepsilon} \equiv \frac{1}{\Omega} \sum_{k=1}^{\Omega} \varepsilon_k. \quad (13)$$

In the strong-coupling limit, the energies E_i fulfill $E_i \gg \varepsilon_k$, and one can expand the Richardson equations (3) in terms of the small parameters ε_k/E_i . This yields sums of the form $\sum_i E_i^{-p}$ which in turn are expanded into a series of inverse powers of the coupling g . The corresponding expansion coefficients can be determined

through recursion relations. We formally extend the results by Yuzbashyan *et al.* [25] and write the ground-state energy as

$$E(\{\varepsilon_j\}) = E^{(1)} + 2N\bar{\varepsilon} + g \sum_{j \geq 2} \sum_{\lambda} \frac{c_{\lambda}}{g^j} \prod_{i=1}^k \overline{(\varepsilon - \bar{\varepsilon})^{\lambda_i}}. \quad (14)$$

Here, N denotes the number of fermion pairs, and

$$E^{(1)} \equiv -N(\Omega - N + 1)g \quad (15)$$

is the leading contribution of order g to the ground-state energy. The sum over λ in Eq. (14) runs over all partitions $\lambda = [\lambda_1, \lambda_2, \dots, \lambda_k]$ of j into integers $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_k \geq 2$ such that

$$j = \sum_{i=1}^k \lambda_i. \quad (16)$$

Let us analyze the ground-state energy (14). The first term is of order g and is quadratic in particle number. In the strong coupling limit, each single-particle orbital has approximately equal occupation $2N/\Omega$, and the second term on the right hand side of Eq. (14) sums the corresponding single-particle energies. The subsequent terms contain ratios of single-particle energies and the pairing strength, and these central moments are invariant under shifts of the single-particle energies.

Yuzbashyan *et al.* estimated that the expansion (14) converges for ratios $(\varepsilon_j - \bar{\varepsilon})/g \approx 1$. They gave explicit expressions for the first two coefficients c_{λ} . Snyman and Geyer [29] corrected a typo in the second coefficient, and Barbaro *et al.* [30] gave an expression for the two fourth-order terms. We confirmed these results by following the steps described in Ref. [25]. The first few coefficients are thus

$$c_{[2]} = -\frac{4N(\Omega - N)}{\Omega(\Omega - 1)}, \quad (17)$$

$$c_{[3]} = \frac{8N(\Omega - N)(\Omega - 2N)}{\Omega^2(\Omega - 1)(\Omega - 2)}, \quad (18)$$

$$\begin{aligned} c_{[4]} &= -\frac{16N(\Omega - N)}{\Omega^3(\Omega - 1)^2(\Omega - 2)(\Omega - 3)} \\ &\times (\Omega^2(\Omega - 1) - N(\Omega - N)(5\Omega - 6)), \end{aligned} \quad (19)$$

$$\begin{aligned} c_{[2,2]} &= \frac{16N(\Omega - N)}{\Omega^3(\Omega - 1)^2(\Omega - 2)(\Omega - 3)} \left[\Omega^2(2\Omega - 3) \right. \\ &\left. - N(\Omega - N) \left(3(3\Omega - 4) - \frac{\Omega}{\Omega - 1} \right) \right], \end{aligned} \quad (20)$$

and higher-order coefficients can be worked out by following the recursion relations given in Ref. [25].

We are interested in the construction of the density functional (4) for the pairing Hamiltonian with ground-state energy E . This requires us to perform a Legendre transform of the ground-state energy (14) with respect to the single-particle energies (i.e. the external potential).

This transformation is done in three steps. First, we compute the occupation numbers

$$n_j \equiv \frac{\partial E(\{\varepsilon_k\})}{\partial \varepsilon_j} . \quad (21)$$

This is most easily done by utilizing the identity

$$\frac{\partial}{\partial \varepsilon_j} \overline{(\varepsilon - \bar{\varepsilon})^k} = \frac{k}{\Omega} \left((\varepsilon_j - \bar{\varepsilon})^{k-1} - \overline{(\varepsilon - \bar{\varepsilon})^{k-1}} \right) . \quad (22)$$

Second, we express the single-particle energies as functions of the occupation numbers. This inversion is most conveniently done order by order in terms of the strong coupling expansion. Third, we have to compute the sum on the right hand side of Eq. (4). To this purpose we employ the identity

$$\sum_{j=1}^{\Omega} n_j \varepsilon_j = \sum_{j=1}^{\Omega} (n_j - \bar{n})(\varepsilon_j - \bar{\varepsilon}) + 2N\bar{\varepsilon} , \quad (23)$$

where

$$\bar{n} \equiv \frac{2N}{\Omega} \quad (24)$$

is the average occupation number.

Let us follow these steps order by order in the strong coupling expansion. In leading order (LO), the ground-energy is

$$E_{\text{LO}}(\{\varepsilon_j\}) = E^{(1)} + 2N\bar{\varepsilon} , \quad (25)$$

and the occupation numbers (5) are

$$n_j = \bar{n} . \quad (26)$$

This expression is independent of the single-particle energies, and the Legendre transformation cannot be performed. The formal reason is, of course, that the energy (25) does only depend on the sum of the single-particle energies (cf. the discussion at the end of Sect. II). In the strong-coupling limit, all single-particle orbitals have equal occupation. Thus, the individual occupation numbers do not depend on the single-particle energies.

In next-to-leading order (NLO), the ground-state energy is

$$E_{\text{NLO}}(\{\varepsilon_j\}) = E_{\text{LO}}(\{\varepsilon_j\}) + \frac{c_{[2]}}{g} \overline{(\varepsilon - \bar{\varepsilon})^2} . \quad (27)$$

The occupation numbers fulfill

$$n_j - \bar{n} = \frac{2c_{[2]}}{g\Omega} (\varepsilon_j - \bar{\varepsilon}) . \quad (28)$$

Note that $c_{[2]} < 0$, i.e. the occupation of orbitals below (above) the average single-particle energy is above (below) the average occupation number. For the inversion, we take the square of Eq. (28) and average over the single-particle orbitals. This yields

$$\overline{(\varepsilon - \bar{\varepsilon})^2} = \frac{g^2 \Omega^2}{4c_{[2]}^2} (n - \bar{n})^2 . \quad (29)$$

Finally, we compute the sum

$$\sum_{j=1}^{\Omega} n_j \varepsilon_j = \frac{2c_{[2]}}{g} \overline{(\varepsilon - \bar{\varepsilon})^2} + 2N\bar{\varepsilon} . \quad (30)$$

Putting all together, we arrive at the density functional in NLO

$$\begin{aligned} F_{\text{NLO}}(\{n_k\}) &= E_{\text{NLO}} - \sum_{k=1}^{\Omega} n_k \varepsilon_k \\ &= E^{(1)} - \frac{g\Omega^2}{4c_{[2]}} \overline{(n - \bar{n})^2} . \end{aligned} \quad (31)$$

In the presence of an external potential, given in terms of single-particle energies ε_j , the density functional thus becomes

$$E_{\text{NLO}}(\{n_k\}) = F_{\text{NLO}}(\{n_k\}) + \sum_{j=1}^{\Omega} n_j \varepsilon_j . \quad (32)$$

The ground-state energy for the system with N pairs is found from the requirement that number-conserving variations of the functional vanish. The corresponding occupation numbers fulfill

$$\frac{\partial E_{\text{NLO}}(\{n_k\})}{\partial n_j} = 0 , \quad (33)$$

and it is understood that the derivative does not act on the N -dependent constants $E^{(1)}$ and $c_{[2]}$ of the functional (31). It is straightforward to check that the solution of this equation yields the energy (27).

For the calculation of the density functional in N²LO we start from the expression

$$E_{\text{N}^2\text{LO}}(\{\varepsilon_j\}) = E_{\text{NLO}}(\{\varepsilon_j\}) + \frac{c_{[3]}}{g^2} \overline{(\varepsilon - \bar{\varepsilon})^3} \quad (34)$$

for the energy, and repeat the three steps outlined above. For the inversion, we raise the expression corresponding to Eq. (28) to the second and third power, and average over single-particle orbitals. We neglect any terms of order $O([(\varepsilon_j - \bar{\varepsilon})/g]^4)$ or higher that are generated in this procedure. This yields two linear equations that express the central moments of occupation numbers $(n - \bar{n})^\mu$ for $\mu = 2, 3$ in terms of the central moments of the energy $(\varepsilon - \bar{\varepsilon})^\mu$. The inversion is straightforward, and the final result is

$$F_{\text{N}^2\text{LO}}(\{n_k\}) = F_{\text{NLO}}(\{n_k\}) + \frac{gc_{[3]}\Omega^3}{8c_{[2]}^3} \overline{(n - \bar{n})^3} . \quad (35)$$

Let us pause for a moment and consider Eqs. (31) and (35), respectively. The strong-coupling expansion of the ground-state energy (14), given in central moments of the single-particle energies, translates into an expansion of central moments of occupation numbers. Clearly, deviations of the occupation numbers from their mean value

\bar{n} increase with increasing value of the ratios $(\varepsilon_j - \bar{\varepsilon})/g$. In the limit of vanishing pairing strength $g \rightarrow 0$, the occupation numbers become discontinuous at the Fermi energy. Note that the density functional is local in the occupation numbers up to N²LO, as only simple sums over occupation numbers appear. Nonlocalities start to appear at N³LO, and we will address this order in what follows.

At N³LO, the ground-state energy is

$$E_{\text{N}^3\text{LO}}(\{\varepsilon_j\}) = E_{\text{N}^2\text{LO}}(\{\varepsilon_j\}) + \frac{c_{[4]}}{g^3} \overline{(\varepsilon - \bar{\varepsilon})^4} + \frac{c_{[2,2]}}{g^3} \left(\overline{(\varepsilon - \bar{\varepsilon})^2} \right)^2. \quad (36)$$

As we will see, the last term in this equation gives rise to the nonlocality in the density functional. Such products of central moments of single-particle energies are ubiquitous at higher orders. For the occupation numbers, we find

$$\begin{aligned} n_j - \bar{n} &= \frac{2c_{[2]}}{g\Omega} (\varepsilon_j - \bar{\varepsilon}) \\ &+ \frac{3c_{[3]}}{g^2\Omega} \left((\varepsilon_j - \bar{\varepsilon})^2 - \overline{(\varepsilon - \bar{\varepsilon})^2} \right) \\ &+ \frac{4c_{[4]}}{g^3\Omega} \left((\varepsilon_j - \bar{\varepsilon})^3 - \overline{(\varepsilon - \bar{\varepsilon})^3} \right) \\ &+ \frac{4c_{[2,2]}}{g^3\Omega} (\varepsilon_j - \bar{\varepsilon}) \overline{(\varepsilon - \bar{\varepsilon})^2}. \end{aligned} \quad (37)$$

We raise this equation to the power two, three, and four, average over single-particle orbitals, and neglect any terms on the right hand sides that are of order $O([(\varepsilon_j - \bar{\varepsilon})/g]^5)$ or higher. The resulting three equations express the central moments of the occupation numbers as nonlinear functions of central moments of the single-particle energies, and the nonlinearities are due to the terms proportional to $c_{[2,2]}$. We invert these equations and neglect terms that are of order $O((n_j - \bar{n})^5)$ or higher. The final result for the density functional is

$$\begin{aligned} F_{\text{N}^3\text{LO}}(\{n_k\}) &= F_{\text{N}^2\text{LO}}(\{n_k\}) \\ &+ \frac{4c_{[2]}c_{[2,2]} + 9c_{[3]}^2}{64c_{[2]}^5} g\Omega^4 \left(\overline{(n - \bar{n})^2} \right)^2 \\ &+ \frac{4c_{[2]}c_{[4]} - 9c_{[3]}^2}{64c_{[2]}^5} g\Omega^4 \overline{(n - \bar{n})^4}. \end{aligned} \quad (38)$$

The second term on the right hand side of this equation is nonlocal in the occupation numbers, since it involves a double sum. This form of nonlocality is, however, rather simple, as the double sum is a product of two individual sums.

We can now generalize the expansion of the density functional to higher orders. The density functional at order j consists of products of central moments of the occupation numbers, and includes occupation numbers

up to the power of j , i.e

$$F(\{n_j\}) = E^{(1)} + g \sum_{j \geq 2} \sum_{\lambda} d_{\lambda} \Omega^j \prod_{i=1}^k \overline{(n - \bar{n})^{\lambda_i}}. \quad (39)$$

Here, λ again denotes the sum over partitions (cf. Eq. (16)), and coefficients d_{λ} are functions of the coefficients c_{λ} in Eq. (14). The functional is nonlocal, but the multiple sums over occupation numbers simply factor into products of simple sums. Thus, the nonlocal structure is rather simple. It is also inexpensive from a computational point of view.

It is interesting to compare the structure of the functional (39) in the strong-coupling limit with the functional (12) from BCS theory. Within the BCS approximation, the nonlocality is limited to the square of a local functional. This suggests that products of multiple local functionals, as they appear in (39), must be corrections of order $1/N$ or smaller. This can be verified by expanding the BCS functional (12) around the strong coupling limit. We thus set $n_j = \bar{n} + (n_j - \bar{n})$ in Eq. (12) and keep only terms up to second order in $n_j - \bar{n}$. The result agrees with the NLO result (31) up to a term $-gN$. This term is recovered when corrections of order $1/N$ to the energy (6) are included (see, e.g. the first term of Eq. (2.16) in Ref. [28]).

V. FROM OCCUPATION NUMBERS TO THE DENSITY

How can one extend presently employed density functionals [31, 32] to include pairing effects? A number of approaches can be found in the literature [9, 33, 34]. Here we follow the direct path that links the occupation numbers to the density. Recall that DFT is built on the ground-state density

$$\rho(x) = \sum_{s=\downarrow, \uparrow} \langle \psi | \hat{\Psi}_s^{\dagger}(x) \hat{\Psi}_s(x) | \psi \rangle. \quad (40)$$

Here, $\hat{\Psi}_s^{\dagger}(x)$ creates a fermion with spin projection s at the position x , and $|\psi\rangle$ denotes the ground state. However, the energy functionals (12) and (39) are based on the occupation numbers n_k that specify the occupation of the single-particle orbitals of the pairing Hamiltonian (1). We denote the corresponding single-particle wave functions as $u_k(x)$ and have

$$\hat{a}_{ks}^{\dagger} = \int d^3x u_k(x) \hat{\Psi}_s^{\dagger}(x). \quad (41)$$

Within Kohn-Sham DFT, the ground-state density (40) is given in terms of the occupation numbers n_{α} of the Kohn-Sham orbitals $\phi_{\alpha}(x)$, i.e.

$$\rho(x) = \sum_{\alpha} n_{\alpha} \phi_{\alpha}^*(x) \phi_{\alpha}(x). \quad (42)$$

Here, $n_\alpha = 2$ ($n_\alpha = 0$) for occupied (unoccupied) Kohn-Sham orbitals in fully paired systems, and we use the convention that Greek indices denote Kohn-Sham orbitals while Roman indices label the single-particle orbitals of the pairing Hamiltonian (1). The occupation numbers n_k are related to the Kohn-Sham orbitals and Kohn-Sham occupation numbers via

$$n_k = \sum_\alpha \langle k|\alpha \rangle n_\alpha \langle \alpha|k \rangle, \quad (43)$$

with

$$\langle \alpha|k \rangle = \int d^3x \phi_\alpha^*(x) u_k(x). \quad (44)$$

Thus, the occupation numbers (43) are functionals of the Kohn-Sham orbitals and therefore nonlocal functionals of the density. The functional derivative of interest is

$$\begin{aligned} \frac{\delta F(\{n_k\})}{\delta \phi_\alpha^*(x)} &= \sum_k \frac{\partial F}{\partial n_k} \frac{\delta n_k}{\delta \phi_\alpha^*(x)} \\ &= n_\alpha \sum_k \frac{\partial F}{\partial n_k} \langle k|\alpha \rangle u_k(x). \end{aligned} \quad (45)$$

Thus, one might add a functional of the form (39) or (12) to commonly employed density functionals [31, 32]. The single-particle wave functions $u_k(x)$ are determined by the pairing Hamiltonian; they can be, e.g., plane waves or shell model orbitals. The nonlocality of the density functional has two sources. The first is the nonlocal structure of the functionals (39) and (12) in terms of the occupation numbers, and the second is due to the relation (43) between the occupation numbers and the Kohn-Sham orbitals.

The use of occupation numbers (43) in a density functional is only new at first sight. The Kohn-Sham kinetic energy

$$\begin{aligned} T &= \frac{\hbar^2}{2m} \sum_\alpha n_\alpha \int d^3x \nabla \phi_\alpha^*(x) \cdot \nabla \phi_\alpha(x) \\ &= \sum_k \frac{\hbar^2 k^2}{2m} n_k \end{aligned} \quad (46)$$

can also be written in terms of occupation numbers n_k of plane wave states. Equation (46) is obtained through integration by parts and by a Fourier expansion of the Kohn-Sham orbitals $\phi_\alpha(x)$ in terms of plane waves $u_k(x)$. Thus, DFT practitioners have dealt with this form of nonlocality for a long time. This insight opens the avenue for more complex (and hopefully more precise) density functionals for nuclei. Recall that the very accurate mass formula by Duflo and Zuker [35] explicitly depends on the number of valence nucleons outside of closed shells. These are occupation numbers of shell-model orbitals, e.g., orbitals $u_k(x)$ from the harmonic oscillator or the Woods-Saxon Hamiltonian. Equation (43) might permit

us to explore and extend this very successful mass formula in the DFT setting.

The main advantage of the functionals (12) and (39) over the HFB approach consists of the conservation of particle number. This is very encouraging, as number projection techniques are numerically expensive and pose practical and theoretical difficulties [36]. However, the Hamiltonian (1) is not realistic, and a constant pairing interaction is a crude approximation for nuclei. Furthermore, the involved sums over single-particle orbitals do not converge for infinitely large model spaces. To avoid divergences, one might introduce a cutoff (e.g., the Debye frequency for condensed matter problems), or utilize regularization and renormalization procedures that relate the coupling g to physical observables [37, 38, 39, 40]. These methods not only cure divergences, they also suggest how to make the density functionals (12) and (39) more realistic. The density functionals of the pairing Hamiltonian are totally symmetric in the occupation numbers n_k . This symmetry, of course, reflects the fact that the pairing interaction (1) is a constant and equally scatters pairs between the single-particle orbitals. This suggests to modify the functional (12) through

$$\sum_k \sqrt{n_k(2 - n_k)} \rightarrow \sum_k w_k \sqrt{n_k(2 - n_k)}. \quad (47)$$

Here, w_k is an orbital-dependent weight or cutoff function. The modified functional still exhibits the hallmarks of pairing, as they are described below Eq. (12); appropriately chosen weight functions w_k also regularize the sums over single-particle orbitals, and should be capable of describing more realistic situations.

VI. SUMMARY

We constructed the density functional of the pairing Hamiltonian. This construction is possible in the strong coupling limit, and within the BCS approximation. In the strong coupling limit, the functional is a multiple product of local functionals that depend on the central moments of the occupation numbers. In the BCS approximation, the functional is arguably the simplest nonlocal and nonanalytical functional that causes an instability of the Fermi surface. Both functionals are based on occupation numbers of single-particle orbitals that define the pairing Hamiltonian. These occupation numbers are themselves functionals of the Kohn-Sham orbitals that define the density. Our results suggest a way to include pairing with particle-number conservation into nuclear density-functional theory.

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